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Data Set

Existing Chemical	:	ID: 3806-34-6
CAS No.	:	3806-34-6
EINECS Name	:	2,4,810-Tetraoxa-3,9-diphosphaspiro[5.5]undecane, 3,9-bis(octadecyloxy)-
EC No.	:	223-276-6
Molecular Formula	:	C41H82O6P2
Status	:	
Memo	:	US HPV WESTON 618 Crompton Corp.
Printing date	:	15.12.2003
Revision date	:	
Date of last update	:	15.12.2003
Number of pages	:	1
Chapter (profile)	:	Chapter: 1, 2, 3, 4, 5, 6, 7, 8, 10
Reliability (profile)	:	Reliability: without reliability, 1, 2, 3, 4
Flags (profile)	:	Flags: without flag, confidential, non confidential, WGK (DE), TA-Luft (DE), Material Safety Dataset, Risk Assessment, Directive 67/548/EEC, SIDS

2.1 MELTING POINT

Value	:	37 - 46 °C
Sublimation	:	
Method	:	
Year	:	
GLP	:	no data
Test substance	:	Chemical name: 2,4,810-Tetraoxa-3,9-diphosphaspiro[5.5]undecane, 3,9-bis(octadecyloxy)- CAS No.: 3806-34-6 Trade name: Weston 618F, 618G Phospites Purity: No data, likely to be technical grade
Reliability	:	(4) not assignable Manufacturer's technical data sheet

22.10.2003 (2)

2.2 BOILING POINT

Value	:	705 °C at
Decomposition	:	
Method	:	other: Calculated using MPBPWIN v 1.40
Year	:	2003
GLP	:	
Test substance	:	Chemical name2,4,810-Tetraoxa-3,9-diphosphaspiro[5.5]undecane, 3,9-bis(octadecyloxy)- CAS No.: 3806-34-6
Reliability	:	(2) valid with restrictions

17.11.2003 (7)

2.4 VAPOUR PRESSURE

Value	:	1.06E-18 hPa at 25 °C
Decomposition	:	
Method	:	other (calculated): MPBPWIN v 1.40
Year	:	2003
GLP	:	
Test substance	:	Chemical name: 2,4,810-Tetraoxa-3,9-diphosphaspiro[5.5]undecane, 3,9-bis(octadecyloxy)- CAS No.: 3806-34-6
Reliability	:	(2) valid with restrictions

18.11.2003 (7)

2.5 PARTITION COEFFICIENT

Partition coefficient	:	octanol-water
Log pow	:	15 at °C
pH value	:	
Method	:	other (calculated): KOWWIN v 1.66

Year	:	2003
GLP	:	
Test substance	:	Chemical name: 2,4,810-Tetraoxa-3,9-diphosphaspiro[5.5]undecane, 3,9-bis(octadecyloxy)- CAS No.: 3806-34-6
Reliability	:	(2) valid with restrictions

22.10.2003 (7)

2.6.1 SOLUBILITY IN DIFFERENT MEDIA

Solubility in	:	Water
Value	:	at °C
pH value	:	
concentration	:	at °C
Temperature effects	:	
Examine different pol.	:	
pKa	:	at 25 °C
Description	:	
Stable	:	
Deg. product	:	
Method	:	other: Calculated using WSKOW v 1.40
Year	:	2003
GLP	:	
Test substance	:	Chemical name: 2,4,810-Tetraoxa-3,9-diphosphaspiro[5.5]undecane, 3,9-bis(octadecyloxy)- CAS No.: 3806-34-6
Result	:	Water solubility = 2.95E-12 mg/L
Reliability	:	(2) valid with restrictions

18.11.2003 (7)

3.1.1 PHOTODEGRADATION

Type	:	air
Light source	:	
Light spectrum	:	nm
Relative intensity	:	based on intensity of sunlight
INDIRECT PHOTOLYSIS		
Sensitizer	:	OH
Conc. of sensitizer	:	1500000 molecule/cm³
Rate constant	:	.0000000001863 cm³/(molecule*sec)
Degradation	:	% after
Deg. product	:	
Method	:	other (calculated): AOP v 1.90
Year	:	2003
GLP	:	
Test substance	:	Chemical name: 2,4,810-Tetraoxa-3,9-diphosphaspiro[5.5]undecane, 3,9-bis(octadecyloxy)- CAS No.: 3806-34-6
Result	:	T1/2 = 0.689 hours

22.10.2003 (7)

3.1.2 STABILITY IN WATER

Type	:	Abiotic
t1/2 pH4	:	at °C
t1/2 pH7	:	at °C
t1/2 pH9	:	at °C
Deg. product	:	No
Method	:	Other
Year	:	2004
GLP	:	
Test substance	:	2,4,810-Tetraoxa-3,9-diphosphaspiro[5.5]undecane, 3,9-bis(octadecyloxy)- Purity: Technical grade Source: General Eletrical
Method	:	Due to the poor water solubility of the test substance, an adequate hydrolysis study could not be conducted. However, the test substance was hydrolytically unstable similar to other organophosphite class of chemicals at all pHs'.
Result	:	
Reliability	:	(2) valid with restrictions

10.21.2004 (6)

3.3.1 TRANSPORT BETWEEN ENVIRONMENTAL COMPARTMENTS

Type	:	fugacity model level III
Media	:	
Air	:	% (Fugacity Model Level I)
Water	:	% (Fugacity Model Level I)
Soil	:	% (Fugacity Model Level I)
Biota	:	% (Fugacity Model Level II/III)
Soil	:	% (Fugacity Model Level II/III)
Method	:	other: Calculation using EPIWIN Level III Fugacity Model
Year	:	2003
Test condition	:	Henry's Law Constant: 8.15E-6 atm-m3/mole (Henrywin program) Vapor pressure: 8E-17 mmHg (Mpbpwin program) MPt.: 46°C (user entered) Log Kow: 15.1 (Kowwin program) Soil Koc: 4.6E+14 (calc by model) 1000 kg/hr emissions to air, water and soil compartments.
Test substance	:	Chemical name: 2,4,810-Tetraoxa-3,9-diphosphaspiro[5.5]undecane, 3,9-bis(octadecyloxy)- CAS No.: 3806-34-6

	Mass Amount (percent)	Half-life (hr)	Emissions (kg/hr)
Air	0.02	1.38	1000
Water	2.39	1440	1000
Soil	28.6	1440	1000
Sediment	68.9	5760	0

	Fugacity (atm)	Reaction (kg/hr)	Advection (kg/hr)	Reaction (percent)	Advection (percent)
Air	8.51E-20	926	18.4	30.9	0.614
Water	1.36E-20	87.5	182	2.92	6.06
Soil	1.22E-22	1050	0	35	0
Sediment	1.32E-20	631	105	21	3.5

Persistence time: 2540 hr
Reaction time: 2820 hr
Advection time: 24900 hr
Percent reacted: 89.8
Percent advected: 10.2

Half-lives (hr), (based upon Biowin (ultimate) and Aopwin):
Air: 1.378
Water: 1440
Soil: 1440
Sediment: 5760
Biowin estimate: 1.964 (months)

Advection times (hr):
Air: 100
Water: 1000
Sediment: 5E+4

Reliability : (1) valid without restriction
22.10.2003 (7)

3.5 BIODEGRADATION

Type : aerobic
Inoculum :
Deg. product :
Method : other: calculated using Biowin v 4.0
Year : 2003
GLP :
Test substance :

Result : MITI Linear Biodegradation Probability = 0.3588
MITI Non-linear Biodegradation Probability = 0.0660

The substance is predicted to be not readily biodegradable

Test substance : Chemical name: 2,4,810-Tetraoxa-3,9-diphosphaspiro[5.5]undecane, 3,9-bis(octadecyloxy)-
CAS No.: 3806-34-6

Reliability : (2) valid with restrictions
22.10.2003 (7)

5. Toxicity

Id 3806-34-6
Date 15.12.2003

4.1 ACUTE/PROLONGED TOXICITY TO FISH

Type	:	
Species	:	
Exposure period	:	96 hour(s)
Unit	:	mg/l
Method	:	other: Calculated using ECOSAR v 0.99g
Year	:	2003
GLP	:	
Test substance	:	Chemical name: 2,4,810-Tetraoxa-3,9-diphosphaspiro[5.5]undecane, 3,9-bis(octadecyloxy)- CAS No.: 3806-34-6
Result	:	LC50 = 2.94E-10 mg/L The LC50 value is above the estimated water solubility of this substance.
Reliability	:	(2) valid with restrictions

22.10.2003 (7)

4.2 ACUTE TOXICITY TO AQUATIC INVERTEBRATES

Type	:	
Species	:	Daphnia sp. (Crustacea)
Exposure period	:	48 hour(s)
Unit	:	mg/l
Method	:	other: Calculated using ECOSAR v 0.99g
Year	:	2003
GLP	:	
Test substance	:	Chemical name: 2,4,810-Tetraoxa-3,9-diphosphaspiro[5.5]undecane, 3,9-bis(octadecyloxy)- CAS No.: 3806-34-6
Result	:	LC50 = 7.76E-10 mg/L The LC50 value is above the estimated water solubility of this substance.
Reliability	:	(2) valid with restrictions

22.10.2003 (7)

4.3 TOXICITY TO AQUATIC PLANTS E.G. ALGAE

Species	:	
Endpoint	:	
Exposure period	:	96 hour(s)
Unit	:	mg/l
Method	:	other: Calculated using ECOSAR v 0.99g
Year	:	2003
GLP	:	
Test substance	:	Chemical name: 2,4,810-Tetraoxa-3,9-diphosphaspiro[5.5]undecane, 3,9-bis(octadecyloxy)- CAS No.: 3806-34-6

Result	:	EC50 = 1.03E-09 mg/L The EC50 value is above the estimated water solubility of this substance.
Reliability	:	(2) valid with restrictions

22.10.2003 (7)

5.1.1 ACUTE ORAL TOXICITY

Type	:	LD50
Value	:	> 10000 mg/kg bw
Species	:	rat
Strain	:	Sherman
Sex	:	male/female
Number of animals	:	10
Vehicle	:	other: vegetable oil
Doses	:	10,000 mg/kg
Method	:	other: US Testing Co., Inc. Method
Year	:	1971
GLP	:	no
Test substance	:	Chemical name: 2,4,810-Tetraoxa-3,9-diphosphaspiro[5.5]undecane, 3,9-bis(octadecyloxy)- CAS No.: 3806-34-6 Trade name: Weston 618 Purity: No data, likely to be technical grade
Result	:	No. of deaths: 0 Clinical signs: None of the animals showed any signs of toxicity at the maximum dose that could be given at a single administration
Test condition	:	Weight of animals: 200 - 220 g Concentration administered: Test material suspended in vegetable oil at a ratio of 2:5 grams of sample/mL of oil Administration method: Gavage Post dose observation period: 14 days
Reliability	:	(2) valid with restrictions Apparently well-conducted study

20.10.2003 (6)

5.1.3 ACUTE DERMAL TOXICITY

Type	:	LD50
Value	:	> 2000 mg/kg bw
Species	:	Rabbit
Strain	:	New Zealand white
Sex	:	male/female
Number of animals	:	10
Vehicle	:	
Doses	:	2000 mg/kg
Method	:	OECD Guide-line 402 "Acute Dermal Toxicity"
Year	:	1994
GLP	:	Yes

Test substance	:	Chemical name: 2,4,810-Tetraoxa-3,9-diphosphaspiro[5.5]undecane, 3,9-bis(octadecyloxy)- CAS No.: 3806-34-6 Trade Name: Weston W618F Lot No.: HBA242 Purity: No data, likely to be technical grade
Result	:	Mortality: No deaths during the study Clinical observations: 2 females had soft stool on day 1. Two rabbits had their colars caught in their mouth during test material exposure and one of these animals had wet red material around the mouth. There were no other clinical findings. Dermal observations: The test material induced very slight to moderate erythema on all rabbits and very slight edema on eight rabbits. Desquamation was present on 8 sites by day 7 and one site by day 14. There were no other dermal findings. Three sites had very slight erythema and/or desquamation at study termination (day 14). Body weights: No remarkable changes or differences in body weights noted during this study. Necropsy: Accessory splenic tissue, a common congenital abnormality in this strain of rabbit was noted for 5 animals. There were no other gross necropsy findings for all examined tissues.
Test condition	:	Age: Approximately 11 weeks old Weight: 2098 – 2240 g Volume administered or concentration: Applied neat Post dose observation period: 14 days
Reliability	:	(1) valid without restriction Guideline study conducted to GLP

20.10.2003 (8)

5.2.1 EYE IRRITATION

Species	:	Rabbit
Concentration	:	10 %
Dose	:	other: unspecified
Exposure time	:	Unspecified
Comment	:	
Number of animals	:	6
Vehicle	:	other: Cottonseed oil
Result	:	slightly irritating
Classification	:	not irritating
Method	:	other: Federal Register, Vol 29, No. 182, p 13009, 17 September 1964
Year	:	1971
GLP	:	No

Test substance	:	Chemical name: 2,4,810-Tetraoxa-3,9-diphosphaspiro[5.5]undecane, 3,9-bis(octadecyloxy)- CAS No.: 3806-34-6 Trade name: Weston 618 Phosphite Purity: No data, likely to be technical grade
Result	:	The test material produced a very mild conjunctival effect in two of the animals which cleared by the second day of observation

22.10.2003 (1)

5.5.1 REPEATED DOSE TOXICITY

Type	:	
Species	:	rat
Sex	:	male/female
Strain	:	other: Charles River albino
Route of admin.	:	oral feed
Exposure period	:	90 days
Frequency of treatm.	:	daily ad libitum
Post exposure period	:	none
Doses	:	300, 1,000, 3,000 ppm
Control group	:	yes, concurrent no treatment
NOAEL	:	> 3000 ppm
Method	:	other: Industrial Bio-Test Laboratories Inc. test method
Year	:	1972
GLP	:	no
Test substance	:	Chemical name: 2,4,810-Tetraoxa-3,9-diphosphaspiro[5.5]undecane, 3,9-bis(octadecyloxy)- CAS No.: 3806-34-6 Trade name: Weston Phosphite 618 Lot no.: 24 Purity: No data, likely to be technical grade
Result	:	Body weight: Statistical comparisons of final body weights and total weight gains revealed no significant differences between test and control rats Food/water consumption: Test rats ate amounts of food comparable to that consumed by control rats. Clinical signs: No untoward behavioral reactions were noted among any of the animals employed in the study. Ophthalmologic findings: Non reported Hematologic findings: No outstanding differences between test and control rats were noted with respect to any of the parameters investigated (hematocrit value, erythrocyte count, hemoglobin concentration, total leukocyte count, differential leukocyte count). Clinical blood chemistry findings: Values for blood urea nitrogen concentration, serum alkaline phosphatase activity, serum glutamic-pyruvic transaminase activity and fasted blood glucose concentration for test rats

compared well with controls.

Urine analysis: No significant differences between the urine of test rats and control rats were observed when urine was analysed for glucose concentration, albumin concentration, pH, specific gravity and microscopic elements examination.

Mortality and time to death: Six deaths occurred during the study. All of these deaths resulted from trauma incurred during the collection of blood samples. These deaths occurred in the control as well as the test groups and were not attributed to the ingestion of the test material.

Gross pathology: No outstanding differences were noted between test and control rats.

Organ weight changes: The only statistically significan difference reported was the liver/body weight ratio for the 3000 ppm males. The authors of the study concluded that the lack of any consistent dietary or sex-related response indicates that the intergroup differences were not related to treatment.

Histopathology: All of the lesions noted in the microscopic examination of tissues were those of spontaneous disease and are not unusual for the albino rat. The most frequent findings were lesions in the trachea and lungs, indicating chronic murine pneumonia. These occurred in the control as well as the treated rats.

Test condition : Test subjects

Age at study initiation: no data

Mean body weight at study inititiation: 99 g (male), 115 g (female)

No. of animals/sex/dose: 15

- Study Design

Vehicle: Standard rat ration

Clinical observations performed and frequency:

Body weight: Measured on the first day of the test and at weekly intervals thereafter. Analysed statistically at the end of the study.

Food consumption: Data were collected individually for five rats of each sex in every group weekly during the study.
Abnormal reactions and death: Recorded daily during the investigation.

Blood and urine: Samples were collected individually from 10 rats of each sex from both the control and the 3,000 ppm groups after 45 and 84 days of feeding for analysis.

Organs examined at necropsy (macroscopic and microscopic): Esophagus, stomach (cardia, fundus and pylorus), small intestine (duodenum, jejunum and ileum), cecum, colon, liver, kidneys, spleen, pancreas, urinary bladder, pituitary gland, adrenal gland, testes, seminal vesicle, ovary, bone marrow, thyroid gland, parathyroid gland, salivary gland, prostate gland, heart,

aorta, lung, lymph node (cervical and mesenteric), skeletal muscle, peripheral nerve, bone (femur), spinal cord, uterus, trachea, eye, optic nerve and brain (cerebrum, cerebellum and pons)

Organ weights: Statistical analyses were conducted upon the absolute organ weights and their corresponding ratios to the weight of the body and brain. An Analysis of Variance was conducted first and any significant effects disclosed by that treatment were further studied by t-tests.

Reliability : (1) valid without restriction
Well conducted and reported study

20.10.2003 (4)

5.5.2 GENETIC TOXICITY 'IN VITRO'

Type	:	Ames test
System of testing	:	Salmonella typhimurium strains TA97, TA98, TA100, TA102 Escherichia coli strain WP2/pKM101
Test concentration	:	0, 0.05, 0.1, 0.2, 9.5 mg/plate
Cycotoxic concentr.	:	
Metabolic activation	:	with and without
Result	:	Negative
Method	:	other: Maron & Ames (1983)
Year	:	1985
GLP	:	no data
Test substance	:	Chemical name: 2,4,810-Tetraoxa-3,9-diphosphaspiro[5.5]undecane, 3,9-bis(octadecyloxy)- CAS No.: 3806-34-6

Result : Dispersing the test substance into solutions of acetone/Tween-80 at doses of 0.2mg – 0.5 mg/plate produced cloudy solutions.

Under these conditions, there was neither an increase in the number of revertant cells, nor any toxicity.

It was judged that the test was negative under these conditions.

Reliability : (4) valid without restriction
Summary of study only available

15.12.2003 (5)

5.5.3 GENETIC TOXICITY 'IN VIVO'

Type	:	Micronucleus assay
Species	:	mouse
Sex	:	male/female
Strain	:	ICR
Route of admin.	:	i.p.
Exposure period	:	24, 48 hours
Doses	:	500, 1000, 2000 mg/kg
Result	:	negative
Method	:	OECD Guide-line 474 "Genetic Toxicology: Micronucleus Test"
Year	:	2003

GLP : yes

Test substance : Chemical name: 2,4,810-Tetraoxa-3,9-diphosphaspiro[5.5]undecane, 3,9-bis(octadecyloxy)-
CAS No.: 3806-34-6
Trade name: Weston 618F
Lot No.: H41425

Result : Effect on mitotic index or PCE/NCE ratio by dose level by sex: See table below.

Genotoxic effects: Negative

Mortality at each dose level by sex:

Pilot toxicity study: No mortality occurred at any dose, up to the maximum tested of 2000 mg/kg.

Main study: No mortality occurred at any dose level during the course of the study.

Clinical signs:

Pilot toxicity study: Piloerection was seen in male mice at 100 and 1000 mg/kg and in male and female mice at 2000 mg/kg and lethargy in males at 1000 mg/kg and in male and female mice at 2000 mg/kg.

Main study: Lethargy was observed in male and female mice at 1000 and 2000 mg/kg and piloerection in males and females at all doses tested. All other mice treated with test or control articles appeared normal during the course of the study.

Bodyweight changes:

Pilot toxicity study: Change in group mean bodyweights ranged from -2.9% (male, 2000 mg/kg) to +0.4% (female, 2000 mg/kg) after 3 days.

Mutant/aberration/mPCE/polyploidy frequency, as appropriate: See table below

Food/water consumption: no data available

Table: Summary of Bone Marrow Micronucleus analysis

Treatment (20mL/kg)	Sex	Time (hr)	No. of mice	PCE/Total Erythrocytes (mean ± SD)	Change from Control (%)	Micronucleated Polychromatic Erythrocytes	
						Number per 1000 PCEs (mean ± SD)	Number per PCEs Scored[1]
Corn oil	M	24	5	0.456±0.07	-	0.6±0.22	6/ 10000
	F	24	5	0.526±0.09	-	0.5±0.35	5/ 10000
Test article							
500 mg/kg	M	24	5	0.451±0.03	-1	0.6±0.22	6/ 10000
	F	24	5	0.465±0.02	-12	0.5±0.50	5/ 10000
1000 mg/kg	M	24	5	0.473±0.04	4	0.5±0.35	5/ 10000
	F	24	5	0.479±0.05	-9	0.5±0.35	5/ 10000
2000 mg/kg	M	24	5	0.447±0.03	-2	0.5±0.35	5/ 10000
	F	24	5	0.485±0.06	-8	0.7±0.27	7/ 10000
CP[2]	M	24	5	0.335±0.03	-27	22.2±2.20	*222/ 10000

50 mg/kg	F	24	5	0.325±0.01	-38	20.4±2.43	*204/ 10000
Corn oil	M	48	5	0.502±0.06	-	0.3±0.27	3/ 10000
	F	48	5	0.483±0.05	-	0.6±0.22	6/ 10000
Test article							
2000 mg/kg	M	48	5	0.471±0.05	-6	0.6±0.22	6/ 10000
	F	48	5	0.467±0.05	-3	0.8±0.27	8/ 10000

[1] *statistically significant, p<=0.05 (Kastenbaum-Bowman Tables).
[2] cyclophosphamide monohydrate

Test condition : Age at study initiation: 6 - 8 weeks old at the initiation of each phase of the study.

No. of animals per dose:
Pilot toxicity study: 2 male mice dosed at 1, 10, 100 or 1000 mg/kg b.w.; 5 male and 5 female mice dosed at 2000 mg/kg.

Main study: Groups of 5 male/5 female mice dosed at 0, 500, 1000, 2000 mg/kg (euthanized at 24 h); Groups of 5 male/5 female dosed at 0, 2000 mg/kg (euthanized at 48 h).

Route: i.p.

Vehicle: Corn oil.

Controls: Vehicle (Corn oil), cyclophosphamide monohydrate (positive).

Clinical observations performed: Clinical signs, mortality, bodyweight

Organs examined at necropsy: none

Criteria for evaluating results: The incidence of micronucleated polychromatic erythrocytes per 2000 polychromatic erythrocytes was determined for each mouse and treatment group. Statistical significance was determined using the Kastenbaum-Bowman tables which are based on the binomial distribution. In order to quantify the proliferation state of the bone marrow as an indicator of bone marrow toxicity, the proportion of polychromatic erythrocytes to total erythrocytes was determined for each animal and treatment group. The test article was considered to induce a positive response if a dose-responsive increase in micronucleated polychromatic erythrocytes was observed and one or more doses were statistically elevated relative to the vehicle control (p<=0.05, Kastenbaum-Bowman Tables) at any sampling time. However, values that were statistically significant but did not exceed the range of historical negative or vehicle controls were judged as not biologically significant. The test article was judged negative if no statistically significant increase in micronucleated polychromatic erythrocytes above the concurrent vehicle control values and no evidence of dose responses were observed at any sampling time.

Criteria for selection of M.T.D.: based on preliminary toxicity study.

Reliability : (1) valid without restriction
15.12.2003

(3)

5.8.1 TOXICITY TO FERTILITY

5.8.2 DEVELOPMENTAL TOXICITY/TERATOGENICITY

(1) Food and Drug Research Laboratories, Inc. (1971) Weston 618 Phosphite Rabbit Eye Irritation Study, Report No: IBL 10201-F

(2) GE Specialty Chemicals, Inc. (2000). Weston 618F, 618G Phosphites, Technical Data Sheet CA-200H

(3) Gudi, R., & Krsmanovic, L. (2003) Bioreliance, Mammalian erythrocyte micronucleus test, Study No. AA77XC.123.BTL

(4) Industrial Bio-Test Laboratories, Inc. (1972), 90-day subacute oral toxicity study with Weston Phosphite 618 in albino rats, Report No. B1704.

(5) Takizawa, Y (1984) Public hygenic Section, Medical Dept., Akita University, Japan, Report No. BWCT-022-5

(6) United States Testing Company, Inc. (1971). Report of Test Number 51044.

(7) US EPA, EPIWIN v3.10, EPI Suite Software, 2000

(8) Wil Research Laboratories, Inc. (1994), Acute Dermal Toxicity Study of Weston W618F in Albino Rabbits, Report No. WIL-202008